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This program was divided into two sections involving two separate kinds of experiments: The first involved an investigation into the possibility of twinning in complex structures by inhomogeneous shears (without shuffles) possibly involving synchroshear, as we found to be important in HfV2. The second was an experimental investigation into the (low) temperature-stress regime within which twins nucleate. We were able to show using high resolution TEM, that the shear is inhomogeneous, since the plane of mirror symmetry is a particular set of planes in the structure. Second we were able to show that shuffles are not involved since shuffling should be a diffusion-like process and should become very sluggish at low temperatures. We did flow stress measurements down to 4K and found that the twinning process is active all the way down to at least 77K, strongly suggesting that shuffles are not part of the process. As a result, we were able to demonstrate for the first time that the synchroshear process actually appears to be the mechanism by which twinning occurs in this material.

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Final Report

Project Title:
Twinning Mechanisms
in
Complex High T_m Intermetallic Compounds

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Executive Summary

This program was divided into two sections involving two separate kinds of experiments: The first involved an investigation into the possibility of twinning in complex structures by inhomogeneous shears (without shuffles) possibly involving synchroshear, as we found to be important in HfV_2 . We suspect that this is quite a general mechanism. The second was an experimental investigation into the (low) temperature-stress regime within which twins nucleate. Both of these programs also involved extensive use of electron microscopy.

The results to be summarized here are fully described in the publications in the attached package of reprints, and therefore the results will only be briefly summarized.

The impetus of the program was the observation that a particular cubic Laves phase compound based on $\text{HfV}_2 + \text{Nb}$ was found to be capable of plastic deformation at room temperature and that the deformation mode is mechanical twinning. This is quite surprising because of the complex atomic arrangement in the Laves phase which would normally be expected to be incapable of such coordinated atomic motions. There are two choices in the usual way of looking at the process: either the homogeneous atomic motions are relatively small during twinning, the same as in fcc materials, but in this case there also must be substantial atomic shuffles, i.e., the interchanging of atoms while the process continues. The other choice is that the homogeneous atomic motions are very large, four times as large as in fcc materials, but such large motions are normally thought to be impossible. We decided that neither way is correct. Rather, the shears are inhomogeneous, such that some atomic positions undergo shear while others move as blocks, the net result of which is a twinning shear.

If this way of looking at the process is correct, then certain predictions can be made about the twinning: If the shear is inhomogeneous, then the plane of mirror symmetry should be a particular set of planes in the structure, and this

was found to be the case, using high resolution TEM. Second, if the twinning process involves shuffles, then these shuffles should be a diffusion-like process and should become very sluggish at low temperatures. We did flow stress measurements down to 4K and found that the twinning process is active all the way down to at least 77K, strongly suggesting that shuffles are not part of the process.

As a result, we were able to demonstrate for the first time that the synchroshear process actually appears to be the mechanism by which twinning occurs in this material. Prior to this work, there had been no experimental work that supported this interpretation.

List of publications from this program (reprints are attached):

Journals

1. "Stability and Thermal Properties of the Cubic Laves Phase Hf₃₀V₅₅Nb₁₅", Scr. Met. et Mat. 28, 331-36 (1993), with F. Chu.
2. "Deformation Twinning in Intermetallic Compounds - the Dilemma of Shears vs. Shuffles", Mat. Sci. Eng., A170, 39-47 (1993), with F. Chu.
3. "Twinning in Intermetallic Compounds - Are Long Sear Vectors and/or Shuffles Really Necessary?", J. Mater. Sci. Technol., 9, #5,, 313-321 (1993), with F. Chu.
4. "Grain Boundary Faceting and Twinning in Complex Intermetallic Compounds", Phil. Mag. A, 69, 409-20 (1994), with F. M. Chu.
5. "High Temperature Applications of Intermetallic Compounds", D. P. Pope and Ram Darolia, MRS Bulletin, 21, #7, 30-36 (1996).
6. "Impurities, Toughness and Intermetallic Compounds: An Overview", Phys. Stat. Sol.(A), 160, 481-486, (1997).
7. "Analysis of Stacking Faults in the Hf-V-Nb Cubic Laves Phase", Scr. Materiala, 37, 713, (1997), David Luzzi.
8. "Deformation Twinning at Low Temperatures in a Hf-V-Nb Cubic Laves Phase", Acta Materiala, 221, 2913, (1998), with David E. Luzzi, G. Rao, and T. Dobbins.

Conferences

9. "Deformation of a HF-V-NB C15 Laves Phase", F. Chu and D.P. Pope, in: High Temperature Ordered Intermetallic Alloys - V, I. Baker, R. Darolia, J.D. Whittenberger and M.H. Yoo, Editors, Materials Research Society, Pittsburgh, PA (1993), pp 561-566.
10. "Growth of Single Crystalline Intermetallic Compounds", C.S. Chang, Z.L. Wu and D.P. Pope, in: Containerless Processing: Techniques and Applications, W. H. Hofmeister and R. Schiffman, Editors, TMS, Warrendale, PA (1993), pp 129-138.
11. "Deformation of a C15 Laves Phase: Twinning and Synchroshear", F.M. Chu and D.P. Pope, in: Structural Intermetallics, R. Darolia, J.J. Lewandowski, C.T. Liu, P.L. Martin, D.B. Miracle and M.V. Nathal, Editors, TMS, Warrendale, PA (1993), pp 637-646.
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13. "Annealing Twins and Grain Boundary Faceting in a C15 Intermetallic Compound", F. Chu and D.P. Pope, in: Twinning in Advanced Materials, M.H. Yoo and M. Wutig, Editors, TMS, Warrendale, PA (1994), pp 415-422.
14. "Twinning in Intermetallic Compounds - Are Long Shear Vectors and/or Shuffles Really Necessary?", F.M. Chu and D.P. Pope, in: Ordered Intermetallics (IWOI '92), T.L. Lin and C.T. Liu, Editors, National Natural Science Foundation of China, Peoples Republic of China (1994), pp. 86-100.
15. "Deformation of C15 Laves Phase Alloys", F. Chu and D.P. Pope, in: High Temperature Ordered Intermetallic Alloys -VI, J. Horton, I. Baker, S. Hanada and R.D. Noebe, Editors, Materials Research Society, Warrendale, PA, USA, (1995), pp. 1197-1208.
16. "Experimental and Theoretical Studies of MV₂ C15 Intermetallic Compounds, (M=Zr, Hf and Ta): Elasticity and Phase Stability", F. Chu, T.E. Mitchell, S.P. Chen, M. Sob, R. Siegl and D.P. Pope, in: High Temperature Ordered Intermetallic Alloys -VI, J. Horton, I. Baker, S. Hanada and R.D. Noebe, Editors, Materials Research Society, Warrendale, PA, USA, (1995), pp. 1389-1394.

17. "Phase Stability and Elasticity of C15 Transition-Metal Intermetallic Compounds", F. Chu, T. E. Mitchell, S. P. Chen, M. Sob, R. Siegl, and D. P. Pope, in Proceedings of the 1995 Hume-Rothery Award Symposium, TMS, Warrendale, PA.
18. "Ductility and Toughness Considerations in Intermetallics", Y. Kimura and D.P. Pope, in Structural Intermetallics 1997, M. V. Nathal, R. Darolia, C. T. Liu, P. L. Martin, D. B. Miracle, R. Wagner, and M. Yamaguchi, Editors, TMS, Warrendale, PA (1997).
19. "Why Are Intermetallic Compounds Brittle?", Y. Kimura and D. P. Pope, Proceedings of the Eleventh International Symposium on Ultra-High Temperature Materials, Ube, Japan, May, 1997.
20. "Affects of Nb on the Deformation of HfV₂-Based Alloys", Y. Kimura, D.E. Luzzi, and D. P. Pope, Interstitial and Substitutional Effects in Intermetallics, R. Noebe, I. Baker and E. P. George, Editors, TMS, Warrendale, PA (1998).
21. "Deformation of a Hf-V-Nb Laves Phase Alloy", Y. Kimura, D. E. Luzzi, and D. P. Pope, to appear in Proceedings of the 3rd International Workshop on Ordered Intermetallic Alloys and Composites, Dong-Liang Lin, Editor, National Natural Science Foundation of China, Beijing, PRC, (1998). (Reprint not yet available)